

Research Highlights from the 1990s

Earth and Environmental Sciences Division

In the 1990s, EES Division made many contributions to national security, environmental quality, and energy security. Highlights of successes during that period are described in this document. The coverage is far from comprehensive, but the examples give an indication of the scope of activities during the 1990s. Attachments list publications and describe industrial collaborations for calendar year 1998, the last year for which a comprehensive list is available.

The web site <http://www.ees.lanl.gov/> and its associated links should be examined for a more comprehensive view of EES Division capabilities and projects. Collaborations with other Los Alamos divisions and research university faculty and students, and our educational outreach projects are included in the descriptions of activities.

EES Division's research successes and their impact are best viewed in the context of six EES scientific and engineering capabilities. These capabilities were deliberately selected as areas for EES Division to concentrate and apply its resources to solve national-scale problems in environmental quality, energy, and national security, as related to the DOE mission. Each capability represents a combination of people, laboratories, and computer codes, all of which are nurtured to help maintain Los Alamos' position as a top research institution. The capabilities receive priority with regard to hiring post-doctoral fellows and permanent staff members. Each capability is considered to be rich in frontier scientific and engineering challenges, with potential for high-impact, refereed journal publications. These capabilities are marketed to customers as a means to solve their problems.

The six capabilities are:

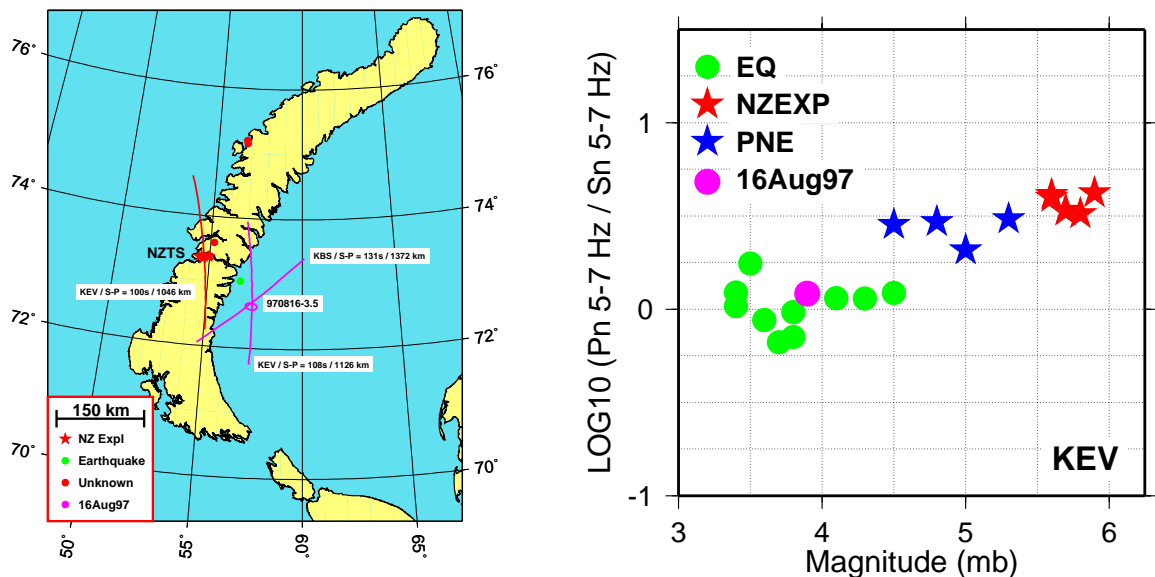
- Seismic and acoustic wave phenomena
- Geomaterials
- Risk assessment methods
- Advanced sensors, technologies, and instrumentation
- Fluid phenomena in earth and environmental systems
- Predictive modeling of earth and environmental systems

1. Seismic and Acoustic Wave Phenomena. Seismic and acoustic signals contain information about the energetic source(s) that created the waves and information about the material properties and the structure along the propagation path between the source region and the receiver. EES Division research in seismic and acoustic wave phenomena includes: 1) developing ground-based seismic and atmospheric infrasound methodologies for detecting and characterizing nuclear tests, especially clandestine nuclear tests; 2) seismic imaging of and modeling of wave propagation through petroleum

reservoirs; and 3) basic and applied science of nonlinear mesoscopic elastic properties of rocks and other materials.

Earthquake/Nuclear Explosion Discrimination. A suspect seismic event occurred near the Russian nuclear test site on the Arctic island of Novaya Zemlya on August 16, 1997. Soon after, the United States issued a *demarche* asserting that Russia had conducted a probable underground nuclear explosion at Novaya Zemlya. Because the 16 August event was recorded only at regional distances and not teleseismic distances, monitoring agencies were not prepared to analyze the event.

- EES scientists used the regional stations KEV in northern Finland and KBS on Spitsbergen to quickly show that the event occurred at least 80 km east of the Russian test site and beneath the Kara Sea.
- They used body waves of previous regional events (earthquakes and explosions) recorded at KEV to show that the 16 August event falls within the regional earthquake population and is separated from the nuclear explosions that have been detonated at the test site and in northwest Eurasia.
- Taking the location and identification evidence together, they confidently classified the 16 August event as an earthquake. Because of this and other studies, the United States subsequently rescinded the *demarche*.



Left: Location of seismic events at or near Novaya Zemlya. The 16 August event was located off shore in the Kara Sea well east of the test site. Right: High-frequency P/S discriminants demonstrated that the event was most likely an earthquake.

Clandestine Nuclear Explosion Detection. EES scientists deploy portable seismic, infrasound, electrical, and videographic equipment in experiments at selected locations across the world to characterize, compare, and contrast seismic signals from earthquakes and explosive sources.

Foremost among these experiments is the seismic monitoring of blasts in a large open-pit coal mine in the Powder River Basin, Wyoming. These blasts have involved as much as 4.5 million pounds of explosives.

- Single-charge explosions, such as clandestine nuclear explosions, can now be identified in the midst of a large mining explosion such as a cast blast.
- These results are being used to develop improved monitoring capabilities for detecting, discriminating, and characterizing underground nuclear tests, especially in Russia, China, and other parts of Asia.

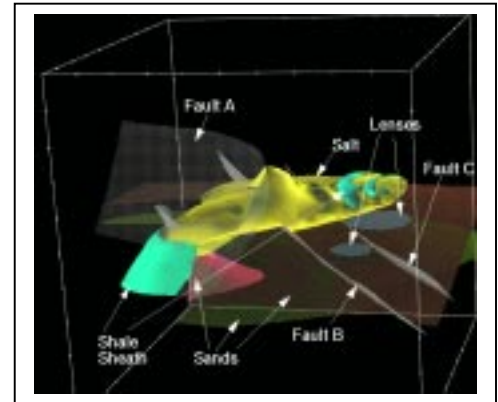


In the photograph above, EES scientists are shown installing seismic monitoring equipment at a Powder River Basin coal mine. The four middle frames are seismic signals synergized with a 4.5 million pound cast blast. The right side of the figure shows time aligned models of the explosive timing effects on the P waves propagated from the source. The models illustrate the complex interference effects generated by the complex mining explosions.

Basic and Applied Seismic Imaging and Modeling. EES scientists have achieved a lead position in seismic imaging and modeling as a result of their ability to perform computationally fast and reliable numerical solutions for the wave equation in heterogeneous media.

Collaborations involve six research universities and 22 oil and gas companies; the scope of the collaboration is important because it has accelerated the pace of the impact of their research on the academic and industrial communities.

- This work demonstrated the usefulness of a 2 Terabyte synthetic seismic data set as a means to achieve improved 3-D seismic imaging through new, faster methods.
- It created an improved method for seismic ray tracing using a technique called “wavefront construction” and implemented it in Kirchhoff migration, the imaging method most commonly used method for imaging by petroleum companies. The resulting migrations are superior to those obtained using Kirchhoff migration with conventional ray tracing.



Test model of diapiric salt layer used in the development of new imaging methods.

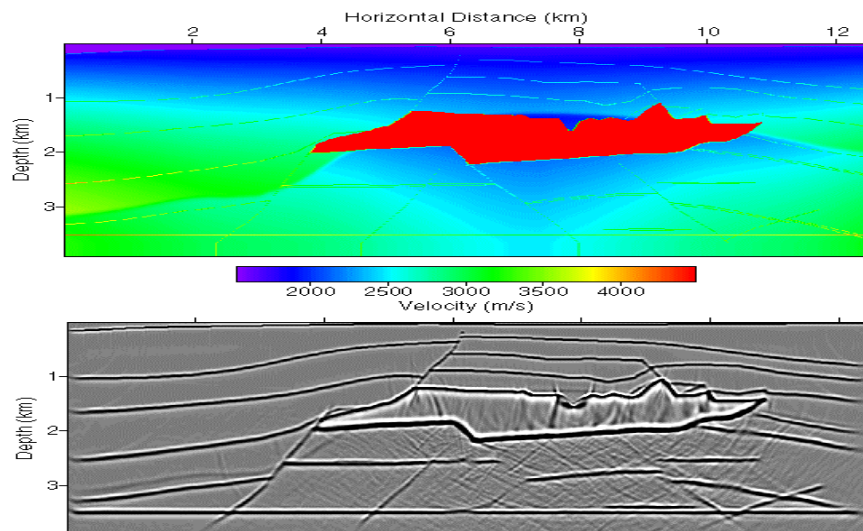


Image Obtained using Extended Local Rytov Fourier Migration

Cross-section (top) and calculated image (bottom) of salt model.

- Developed three new methods for solving the one-way wave equation, one based on a local application of the Born Approximation, one on a local application of the Rytov approximation, and one on an extension of the Born approximation that we call quasi-Born approximation.

Basic and Applied Research in Nonlinear Mesoscopic Elasticity (a New Field of Geophysics). A rock is highly nonlinear material due to the huge volume of discontinuities it contains in the form of microscopic cracks and contacts between grains. The discontinuities make the material compliant in a highly nonlinear manner and classical perturbation theory does not describe the nonlinear behavior adequately. EES scientists have been studying the nonlinear properties of rocks and other earth

materials for approximately 14 years. Today, they and their colleagues are the world leaders in both basic and applied research in this study area. Their work has created a new field of geophysics.

- Recognition of that work is appearing in such forms as an article in the April 1999 issue of *Physics Today*, including the cover.
- Damaged material, such as steel or glass, was discovered by EES scientists to also have a large nonlinear response. A single macrocrack or a volume of microcracks in glass or steel induces a nonlinear behavior similar to rock, as it turns out. This is true, for example, of concrete, of aircraft and automobile components, and of steel beams.
- Consequently, results of their research on the nonlinear properties of earth materials is having fascinating applications in areas such as nondestructive testing of assembly line components and nuclear weapons components.



2. Geomaterials. EES Division's geomaterials capability emphasizes a mechanistic, first-principles to understanding the microscopic to macroscopic characteristics of the material—not an empirical approach. Materials of interest include concrete, natural minerals such as clays and zeolites, nuclear and chemical waste forms, and materials of the deep earth. Applications include creating concrete with superior durability, strength and new uses; improved radioactive waste forms; and acquiring knowledge of the health effects of minerals.

Geomaterials Approach to Improving Concrete Durability. Concrete and other cement-based composites are arguably the most important materials on which the infrastructure of civilization depends. Because of their complexity and heterogeneity, however, these materials are typically studied empirically, which severely limits one's ability to predict their behavior over long periods of time or under conditions that cannot be reproduced in the lab. EES scientists are developing a novel mechanistic, geomaterials model for the chemical and physical processes that determine the durability of these materials. Such a model will allow a systematic approach to tailoring a design for improved durability and performance.



- Developed a patented, R&D100 Award winning field analysis kit.
- Identified a novel biogeochemical mechanism for one of the major degradation mechanisms in concrete

CHEMIN: A Novel Tool For Combined Compositional and Mineralogical Analysis.

Characterization of earth and planetary systems requires determining both chemistry and mineralogy. EES scientists have developed a novel, miniaturized instrument (CHEMIN) optimized for the simultaneous characterization of both composition and the types of crystalline phases.

- The instrument was patented and became an R&D100 Award winner.
- It allows remote analysis of materials for applications ranging from hazardous Hanford tanks to Martian soils.
- Industrial interest includes on-line use in the production of cements to improve efficiency and quality.



Advanced Algorithms for Structural Interpretation of Powder Diffraction Data. Many earth materials are complex mixtures and are often structurally disordered. Characterization of these materials was impossible with traditional techniques. EES scientists developed algorithms and theoretical models that allow quantitative evaluation of complex and disordered earth materials.

- Pioneered quantitative mineralogical analysis using Rietveld techniques (in collaboration with LANSCE);
- Developed novel algorithms for quantitative structural interpretation of disordered layered materials; and
- Developed new structural models for clays and opal, two of the most important materials in earth environments ranging from oil reservoirs to Yucca Mountain.

Predicting Volcanic Eruptions by Changes in Gas Composition.

EES scientists developed a unique understanding of the changing composition of volcanic gases on the scale of days using a combination of direct sampling techniques and a novel remote sensing method. Ratios of specific gas species change distinctly in the days prior to eruptions.



- This was the first use of passive infrared spectroscopy (*Nature* article) for the remote measurement of dynamic changes for multiple gas species.
- It extended the distance for land-based monitoring of gas changes to 17 km, allowing a safe buffer.

3. Risk Assessment Methods. Risk assessments are being applied to better understand ecosystems and ecological risks, and to understand volcanic hazards. Ecological risk assessments involve integrated approaches using bioindicators, remote sensing, field experiments, and modeling; all designed to understand the dynamic response of ecosystems in arid/semiarid woodlands and grasslands to climate change, land use change, and other human activities. Volcanic eruptions are a leading natural hazard causing numerous deaths and property loss. A probabilistic-based volcanic hazard methodology has been developed and applied to the Yucca Mountain Site and to Japan.

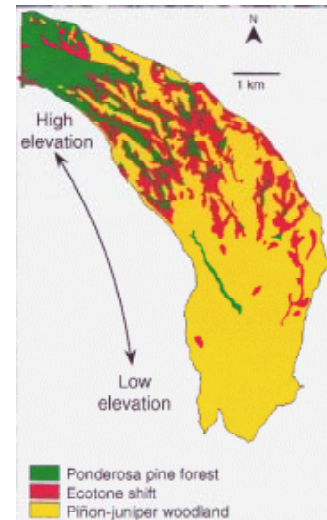
Ecological Risk Assessments at Defense Facilities. A more fundamental basis for ecological risk assessment can be achieved by integrating laboratory studies, field experiments, and landscape-level biological monitoring. This integrated approach is used to measure ecological risk with abiotic characterization results and demographic models to characterize ecological risk at multiple spatial scales. The development of non-lethal sensitive indicators of ecological health will lead to more rapid delineation of problem remediation areas that are biologically amendable. Research successes using this approach are in two areas.

- At Aberdeen, Jefferson, and Yuma Proving Grounds, ecological risk assessments for the US Army showed that there is little risk of adverse health effects to ecological receptors from the exposure of the receptors to depleted uranium fragments in soils.

- At Los Alamos a bluebird nest box biomonitoring network was established. It is one of the largest such biomonitoring networks in the US for evaluating cumulative effects of contaminants and other environmental stress on wild populations.

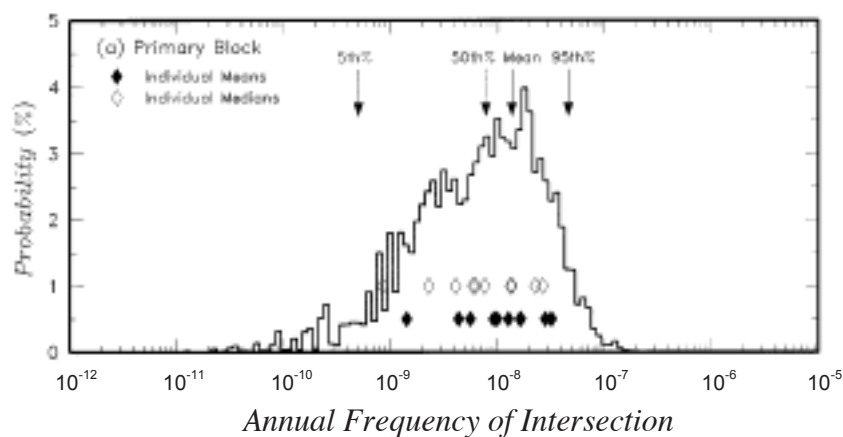
Response of Arid and Semiarid Ecosystems to Climate Change. The pinyon-juniper woodlands and ponderosa pine forests covering much of the Laboratory area and surrounding region have been studied intensely by EES scientists as part of their technical support for environmental clean-up activities. The results continue to provide a scientific basis for decisions associated with the clean-up operations, but other benefits from this work are extending far beyond operational clean-up needs.

- A shift in the ponderosa pine forest/ pinyon-juniper woodland ecotone (boundary between two ecosystems) during the 1950s drought was discovered and found to be more than 2 km in less than 5 years. (See diagram to right). This is the most rapid landscape-scale ecotone shift in response to climate change ever documented, and it attracted enough interest to be published in the *Proceedings of the National Academy of Sciences*.
- Knowledge of ecosystems within the grassland-forest continuum acquired during this work strengthens EES Division's ability to pursue program development to support research related to carbon sequestration using arid and semiarid systems. This is especially important given the fact that arid and semiarid lands comprise approximately one-third of the land surface of the Earth.
- EES scientists created the most intensely instrumented pinyon-juniper woodland plot in existence, and through it discovered the heretofore-unknown importance of shallow subsurface flow (interflow) on water budgets in semiarid environments. They also developed theoretical models for erosion rate transitions. The erosion rate transition models have been used by the Bandelier National Monument to mitigate erosion impacts to archeological sites and by Los Alamos as a possible means for mitigating contaminant transport and designing more stable landfill covers.



Quantitative Volcanic Risk Assessment at the Yucca Mountain Site. Preliminary calculations by EES scientists in the early 1980s showed that the probability of disruption of the Yucca Mountain site by volcanism is less than about 4×10^{-8} per year. Continuing work through the 90s demonstrated the viability of this estimate, but the volcanism issue remained contentious largely due to significant uncertainty in interpreting regulatory requirements for a repository. Therefore, a new analysis was undertaken.

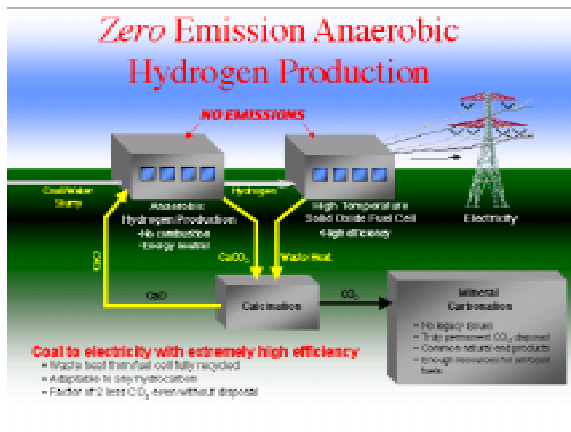
- A summary report of volcanic hazards for Yucca Mountain was completed in 1995 site and gave an estimated mean probability of magmatic disruption of 1.9×10^{-8} per year.
- A panel of 10 internationally recognized experts in volcanism convened in 1996 estimated a mean probability of magmatic disruption of 1.5×10^{-8} per year, thus providing strong confirmation of the 1995 analysis by EES scientists.
- Shortly thereafter, the EES Division scientific approach to volcanic hazard analysis received national recognition through an editorial article in *Science* magazine. Largely as a result of this success, the Japanese repository program funded EES Division to assist in evaluating the volcanic risk to a geologic repository in Japan.



The figure above shows a probabilistic volcanic hazard analysis of the annual frequency of magmatism intersecting the area covered by a repository at Yucca Mountain. (a) Aggregate distribution and median and means for individual expert hazard models for the “Primary Block” case. (b) Range for 5th to 95th percentiles for results from individual expert hazard models compared to range for aggregate distributions.

4. Advanced Technologies, Sensors, and Instrumentation. EES Division continues a tradition to develop, test, and promote new concepts for environmentally benign energy production, to combine science and engineering to create advanced drilling technologies, and to develop new sensors and data acquisition systems for atmospheric sciences research.

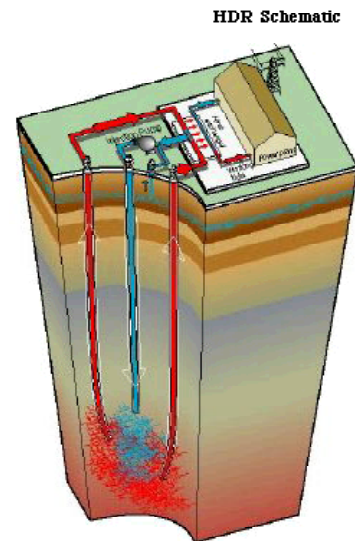
Cradle to Grave Carbon Management Concept. The stability of the world’s economy depends on abundant energy. For economical reasons, the global energy supply has been, and in all likelihood will be continue to be, dominated by fossil fuels, which are far from exhaustion. Limiting energy use to curtail carbon dioxide emissions is likely to stifle the US economy and will certainly leave the vast majority of the world in poverty, as energy use is the enabling agent for wealth. Yet, if left unchecked, the atmospheric concentration of carbon dioxide will double in the next 50 years as poorer nations of the world seek the standard of living enjoyed by today’s richer nations. This



- doubling will take atmospheric carbon dioxide levels higher than at any time in the past 10 million years. However, a Los Alamos concept might provide an answer to this apparent dilemma.

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- Coal to electricity with extremely high efficiency**
- Recycle heat from fuel cell fully recycled
 - Adaptable to any hydrocarbon
 - Emission of 2 less CO₂ per unit of electricity
- Mineral Carbonation**
- No legacy issues
 - Total permanent CO₂ disposal
 - Common natural products
 - Enough resources for centuries
- Los Alamos scientists are pioneering the concept for a zero emissions coal-fueled power plant wherein a carbon dioxide acceptor process for hydrogen production is coupled with high-temperature solid oxide fuel cells.
 - Carbon dioxide is permanently sequestered through an enhanced mineral carbonation process using industrial, aboveground processes or by the injection of supercritical carbon dioxide into appropriate reactive geological strata.
 - This is a concept allowing the continued use of abundant fossil fuels, necessary for economic prosperity, while simultaneously maintaining the natural environmental balance by eliminating carbon dioxide emissions.

Scientific and Engineering Feasibility of Heat Mining. The technology to mine the heat from the hot rock beneath the surface of the earth was conceived, developed, and demonstrated at Los Alamos between the years of 1970 and 1996. Conceptually, hot dry rock (HDR) heat mining is quite simple. Water is pumped into hot, crystalline rock through an injection well; the water becomes superheated as it flows through open joints in the hot rock reservoir, and the water returns to the surface through production wells where heat is extracted by conventional heat exchangers. The same water is then recirculated to mine more heat. The key element in successful heat mining is the use of hydrofracturing to create an engineered system of permeable joints to form a reservoir in a hot body of otherwise impermeable rock.



- The creation of a reservoir to mine the earth's heat was achieved at the Los Alamos Fenton Hill site in 1995 when 4 megawatts of thermal power was routinely produced during an industrial-scale field experiment.
- Energy was extracted for a total of 11 months in three long and several short test periods. During a typical 2-month flow test segment, the fully automated plant produced power continuously at a rate calculated to be on the order of 3-4 times that required to operate the system.

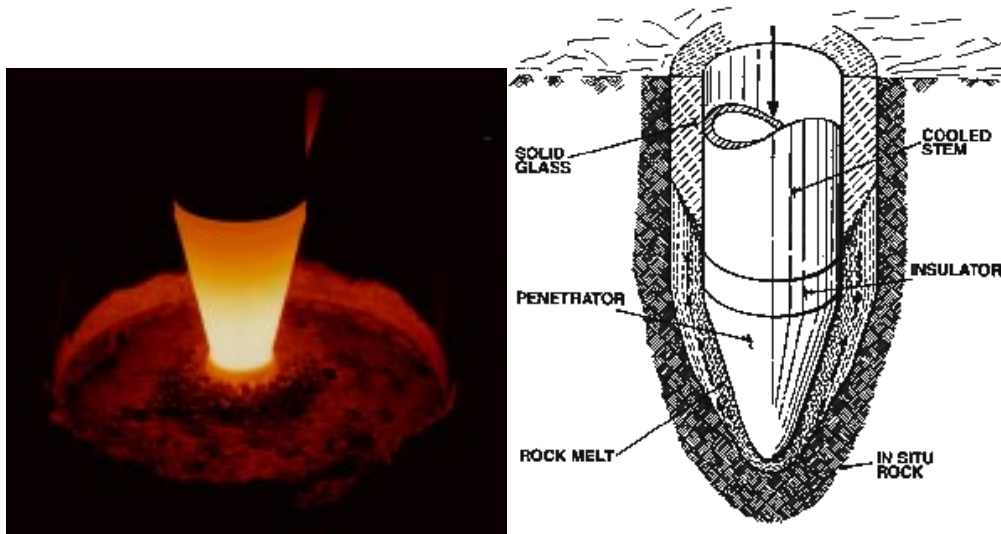
- Since 1995, HDR work in the United States has concentrated on the consolidation of data and understanding of data from the Fenton Hill experiments. Modeling of Fenton Hill data, for example, indicated that production from the large reservoir could have been sustained for more than 40 years without a decline in the production temperature.
- Los Alamos continues to be recognized worldwide as the leader in HDR technology and its supporting sciences. This work led directly to the creation of newer and deeper HDR reservoirs in other parts of the world, and the establishment of HDR activities in Europe, Japan, and Australia. Continued concerns over global warming or the return of high-energy prices could bring a rapid return of interest in HDR.

Microdrilling and Rock Melt Drilling. EES Division has a long history of creating new drilling technologies to gain access into the deep subsurface and into soil-like and rock-like material. Microdrilling technology and rock melting drilling technology are two recent successes. These technologies are leading to new ideas for basic research. In addition, they have the potential for revolutionizing the scope and quality of information that can be collected in the subsurface for a wide range of applications in oil and gas exploration and environmental clean-up, and in national security. Microhole technology is viewed by the external community as a totally Los Alamos innovation. We are the only national laboratory with such a broad integrated involvement in this technology. A forthcoming article in *World Oil* and a recent article in the *London Financial Times* indicates the impact our microhole technology is having.

- In collaboration with five petroleum companies, EES scientists have undertaken an integrated microhole program directed toward miniaturization and testing of bottomhole coiled-tubing drilling assemblies, automation of drilling controls, miniaturization of geophysical logging tools, and incorporation of emerging sensor technologies in borehole instrumentation packages.
- In 1999, four 2-3/8-inch-diameter microholes were successfully drilled and cased to depths of up to 500 ft using an experimental coiled-tubing drilling platform, and it was demonstrated theoretically that 1-3/8-inch microholes can be drilled to 10,000 ft.
- A micromachined accelerometer, a member of the class of sensors called microelectromechanical systems (MEMS), was successfully tested. Its performance already approaches that of conventional accelerometers.

Rock melting was invented by Los Alamos in the early 1960s as a unique method of penetrating rock and soil by melting instead of traditional drilling, which is based on mechanical breakage. Rock melting continued to be developed in the mid 1970's primarily for exploration and development of geothermal resources. But with waning interest in geothermal energy, research on rock melt drilling ceased in 1976. Recently, however, because of some of the unique features of this rock penetration method, there has been renewed interest for specialized applications, and over the last two years

corporate knowledge of the technology acquired during the 1960s and 70s was recovered and the technique was extended.



(The figure above shows a melting-consolidating penetrator entering unconsolidated rock (left) and schematic representation of penetrator (right).

In rock melt drilling, a pointed refractory tip is electrically heated to about 1500° C and thrust into the rock. The rock is partially melted and the melt is forced into the natural porosity of the rock, forming a glass borehole lining that supports the hole open after the hot tip is removed. Since there is no mechanical breakage of rock, the drill is inherently very quiet. Because the drill forms its own hole support (the glass lining) as it goes, there is no need to place tubular casing, and therefore the method is particularly effective in the soils and unconsolidated rock normally encountered at shallow levels underground. Finally, since no rock cuttings are produced, conventional drilling fluids (muds) are not required.

- Applications currently being evaluated include the feasibility of rock melting for stabilization of deep wells, a problem that costs the petroleum industry about \$5B/yr world-wide, and deep drilling on Mars to sample the subsurface hydrosphere and search for extant life.
- For the Martian drilling, we are funded by NASA to evaluate rock melting for this exciting mission. The thermal drilling is of particular interest because of the natural sterilization and planetary protection capability it provides, which is a key concern for this mission.
- Rock melting can also address some special requirements of defense and intelligence applications that we are currently funded to investigate.

Atmospheric Radiation Monitoring Sites in the Tropical Western Pacific. The DOE Atmospheric Radiation Measurement (ARM) program's first decade has been concerned largely with the development and installation of field sites to monitor solar and terrestrial radiation, with emphasis on the role of clouds in modifying these two radiation streams, in order to improve our understanding of the role of clouds in climate. ARM's emphasis is on three climatic regimes (midlatitude continental; tropical marine; arctic—at sites in Oklahoma, the Tropical Western Pacific, and the North Slope of Alaska, respectively) has provided instrument specialists with a variety of technical challenges.

- EES scientists have been responsible for the development of the sites on tropical atolls in the equatorial western Pacific basin since the program's inception, and now has two sites (on Manus Island, Papua New Guinea and in the Republic of Nauru) operational.



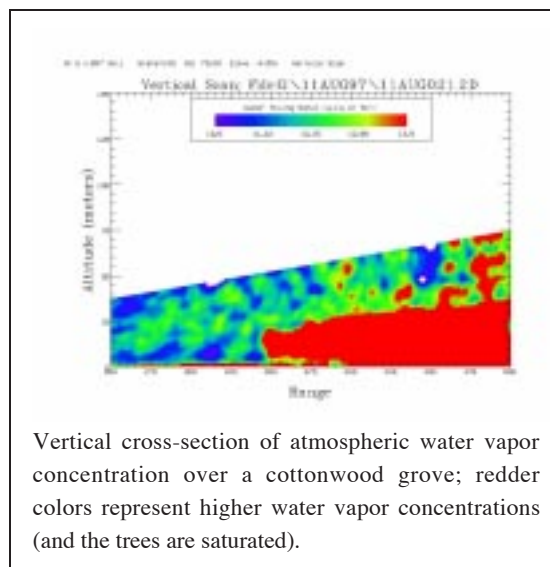
Panoramic view of the ARM site in the Republic of Nauru, constructed, managed, and operated by the LANL Tropical Western Pacific Program Office (TWPPPO).

- In addition to the technical challenges of the instruments involved, the logistical challenges of these remote sites are also significant, but have been overcome. The role of EES scientists is mainly instrument integration and data system development and integration with the instrument packages.
- The experience gained through this effort, however, is significant and offers Los Alamos an opportunity to become a resource for other field efforts—both within the DOE complex and externally.

Development and Application of a Mobile, Scanning Raman Lidar System. Laser applications have a long history at Los Alamos and one of the more innovative of these has been the development of a mobile, scanning Raman lidar system. Unlike backscatter lidar systems, which detect the presence of atmospheric scatterers (from dust to insects to birds) by measuring photons returned by reflections, a Raman system measures photons emitted by stimulated water vapor molecules in the atmosphere. The system's scanning capability thus makes it possible to acquire three-dimensional images of the distribution of atmospheric water vapor. Because of laser power requirements, ranges are limited, but resolution is sufficiently high to allow imaging of structures associated with very small-scale atmospheric turbulence. The combination of these measurements with the simulation

capabilities of HIGRAD presents an extremely powerful tool for understanding the behavior of the atmospheric surface layer and its interactions with the underlying vegetation or other surface layer and its interactions with the underlying vegetation or other surface characteristics.

- A two-dimensional, lidar-derived image of evaporation from the top of a cottonwood grove was acquired during the Semi-Arid Land-Surface-Atmosphere (SALSA) Experiment in the San Pedro River basin of southern Arizona (shown below). The large red area is the cottonwoods themselves, and the red “blobs” over the trees show the structures of the very small-scale turbulence responsible for the evapotranspiration from the grove. Also, it can be seen that evapotranspiration over the adjacent grassland (to the left of the trees) is considerably lower than that over the grove.
- The LANL Raman lidar system is currently a research instrument—that is, a prototype—but there exists some potential for the construction and marketing of an operational version. Both the Bureau of Land Management and of Reclamation have interests in water resource issues, and this instrument is a powerful tool to aid in monitoring surface-atmosphere exchanges. In addition, the system is becoming known throughout the broader atmospheric sciences community as a tool for probing the structure and mechanisms of atmospheric turbulence.



5. Fluid Phenomena in Earth and Environmental Systems. EES scientists use combinations of computational, experimental, and observational techniques to understand fluid flow and mass transport in porous and fractured earth materials and in the earth’s atmosphere. Interests are in multiphase, multicomponent, reactive fluid flow in groundwater unsaturated zones and saturated zones, in petroleum reservoirs, and in hydrothermal/geothermal systems. In addition, fluid flow in the earth’s atmosphere is studied at the microscale (10’s - 100’s m), around buildings, for example, and the mesoscale (1-1000 km), over small to regional terrains. Climate, global atmospheric chemistry and contaminant transport are studied at all scales.

The foremost historical application of this capability—as it relates to the solid earth—was to assure that the highly radioactive gases and particles produced by the underground detonation of a nuclear weapon was entirely contained underground. With the cessation of underground nuclear testing, this application is no longer necessary.

Containment of Underground Nuclear Tests. Since the inception of the Containment Program at Los Alamos in 1971 and continuing until the beginning of the current testing moratorium, Los

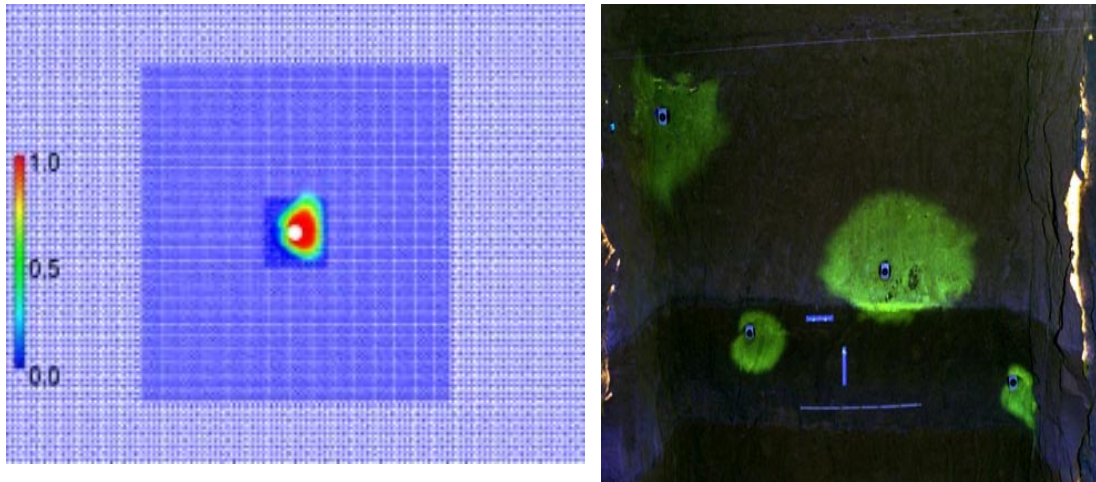
Alamos conducted over 150 tests at the Nevada Test Site without a single radioactive release to the environment. To best of our knowledge, this perfect record is unsurpassed by any other organization or nation. It was made possible by a combination of careful geologic characterization, detailed geophysical analysis, and the development of a unique understanding of nuclear explosion phenomenology. When the program began, the factors that led to containment success or failure were very poorly understood. Over the years, through careful analysis and modeling of event phenomena, including cavity expansion, residual stress formation, and collapse, ground motion and spall, and flow of radioactive gasses in the stemming, EES Division scientists were able to develop a greatly improved understanding of processes that impact containment, such as stress wave propagation, hydrofracture, and porous flow. Effective and robust containment designs based on this knowledge provided the DOE with high confidence that all containment concerns had been addressed and that complete containment would be effected. Despite increasing environmental sensitivities during the later years of the test program, the fundamental understanding of explosion phenomenology and the proven containment design capability allowed EES scientists to address these concerns and the DOE to continue underground testing. Since the cessation of testing, the capabilities that were developed for the containment program have been used to address other important national security issues. These include worldwide monitoring for the detection and characterization of evasively conducted nuclear explosions, and developing the technology for finding, characterizing, and defeating hard and deeply buried targets around the world.

Evaluation of the Yucca Mountain Site. Yucca Mountain, located on the western edge of the Nevada Test site, is being characterized by the DOE as the location for disposal of high-level nuclear waste (commercial spent fuel and defense high-level waste). EES Division has a nearly 20-year record as the prime organization successfully analyzing issues related to modeling radionuclide transport in the groundwater system, the mineralogic setting, and volcanic hazards. In addition, EES Division, since 1993, has had prime responsibility for planning and implementation of the underground testing program in the 5-mile-long Exploratory Studies Facility, the Cross Drift Facility and at the Busted Butte test site.

The Busted Butte test has been a major success for EES Division. The test involves the use of radionuclide and colloid analogs consisting of a mix of conservative and reactive tracers and polystyrene microspheres. An integral part of the test is a computational model that can capture the detailed, complex physical processes, and a numerical grid that can capture the high-resolution spatial configuration of the test block.

- EES scientists have used FEHM (see below) to positively identify and capture the physical mechanisms driving flow and transport in the Busted Butte system.
- Tracer breakthrough results from collection boreholes combined with predictive modeling results on these tests indicate a complex behavior of fracture-matrix interaction is responsible for the transport behavior of solutes from the base of the Topopah Springs formation into the hydrologic Calico Hills. The match between the FEHM-modeled transport away from an injection borehole

(below left) and observed transport away from four injection boreholes (below right) is remarkable.



As the Yucca Mountain Project moves toward a site suitability determination in 2001 and, if suitable, license application to the US Nuclear Regulatory Commission in 2002, EES Division expects to continue to play a key leadership role in the testing program in support of these key milestones to solve an important national problem.

Lattice Boltzmann Methods in Porous Media Flow and Transport. There are many circumstances under which humans want to remove fluids existing below ground in the pore space of the porous rock. Three potential reasons for such removal are obtaining drinking water, removal of a contaminant from an aquifer, or extraction of oil or gas from a reservoir. Scientists from the Laboratory and Mobil Oil have developed and applied a novel numerical approach, the lattice Boltzmann (LB) technique, to model fluid flow in porous media systems. The LB method applies known, fundamental, physical processes governing fluid movement and fluid/solid and fluid/fluid interactions, and is not based on empirical assumptions, as are traditional methods. The basic theory behind the LB method demonstrates that fluid behavior can be simulated using "particles" through simple movement (advection) and interaction (collision) of such particles on a grid that defines the pore space. The way these fluid packets are constrained to move and collide is such that when the entire grid is considered, the overall response exactly recovers the macroscopic hydrodynamic equations that describe fluid behavior in the subsurface. One of the major strengths of this modeling approach is that it is particularly well-suited for massively parallel computer architectures. The LB model won an R&D100 award in 1994, and its Lattice Gas pre-cursor won an R&D100 award in 1988.

Modeling Codes FEHM and GEOMESH. FEHM (Finite Element Heat and Mass Transport), developed by EES Division, is arguably one of the most powerful and versatile groundwater flow and transport codes in existence. FEHM's capabilities range from multiphase flow to multi-species

radionuclide transport, colloid movement, particle tracking, and more. GEOMESH is one of the most flexible mesh generating tools available. GEOMESH is able to very accurately represent complex stratigraphy, utilizing as much known information as is available.

- Coupled, these codes are able to address the most complex, challenging issues in subsurface flow and transport.
- Utilizing the power of FEHM and GEOMESH, EES Division scientists have solved many questions at many sites related to groundwater flow and transport.
- FEHM is becoming more widely recognized and utilized outside of LANL. Consultants, researchers at other national laboratories and university researchers are using FEHM.
- FEHM could, potentially, be licensed for purchase.

Self-Consistent Model of the Carpinteria Reservoir. The oil and gas program in EES Division has strengthened core competencies at the Laboratory and has helped domestic independent oil and gas producers remain competitive. As major oil producers continue to concentrate their efforts on their more profitable overseas properties, many are selling some of their domestic US properties. This is creating opportunities for the approximately 8000 independent oil and gas producers in the US, but many of the domestic properties being acquired by the independents from the majors have marginal economics. The use of advanced computer modeling to predict the flow of oil and gas in the reservoir is required to make them profitable. This advanced computer modeling is often beyond the reach of independent producers. But EES scientists demonstrated that it is possible to bridge the gap when, in the late-1990s, they developed a web-based system designed to deliver advanced reservoir management software to independents and helped with the completion of a redevelopment plan for the Carpinteria Offshore Field, located near Santa Barbara, California.

- As part of this project, EES scientists and an independent oil and gas producer combined advanced modeling and simulation, working through the Internet, to create the first self-consistent model of the Carpinteria Oil Reservoir.
- They demonstrated virtual enterprise computing, years ago at a time when the Internet was evolving into the World Wide Web. This was before business models for the WWW had been conceptualized, as is now the case in almost every business sector.
- In 1998, the Carpinteria Oil Reservoir model was used to guide the drilling of six new wells that today produce at the rate of 850 barrels per day, more oil than the other 75 old wells in the field combined. This was the tangible result of the effort.

The Carpinteria success should be viewed in the context of a larger programmatic success spanning more than 10 years. EES Division pioneered the current DOE model for collaborative research with

the oil and gas industry in 1988 when it joined with Sandia, and later with the other DOE labs, to form the Natural Gas and Oil Technology Partnership. In this model, industry collaborates with national labs, offers opinions to DOE about program directions, and influences the direction of national laboratory research to solve important industry problems.

Stochastic Reservoir Simulation. A recent advance in our capability for predicting subsurface fluid flow is the development of an approach that inherently accounts for heterogeneity and uncertainty in the geologic media. Previous approaches have used a deterministic code like FEHM, running numerous times on different statistically correct realizations of the geologic media to generate an ensemble (or probability distribution) of results. The new technique casts the governing equations as moment equations, so that only a single solution is needed to derive the probability distribution of flow results.

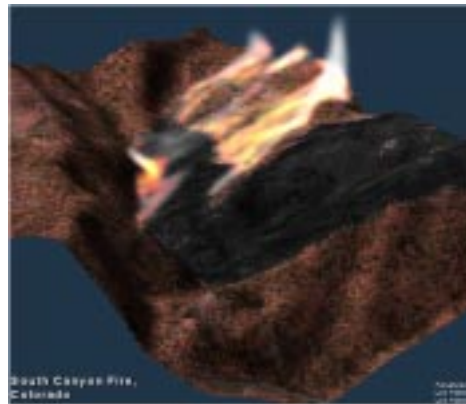
- Already this technique is garnering attention in the environmental and petroleum reservoir communities and we expect it to soon be applied to many real-world problems.
- In addition, we are exploring the coupling of the moment equation technique to probabilistic environmental risk assessment tools.

Atmospheric Flows at Micoscales, Mesoscales, and Regional Scales.

This work was originally motivated by the need to improve understanding of atmospheric flows over the extremely complex terrain of the Los Alamos site. It has grown in sophistication in parallel with the growth in computing power available. Currently, it involves efforts to improve the representation of turbulent flow in regions of high gradients and to include in these computations real-world physics and chemistry.

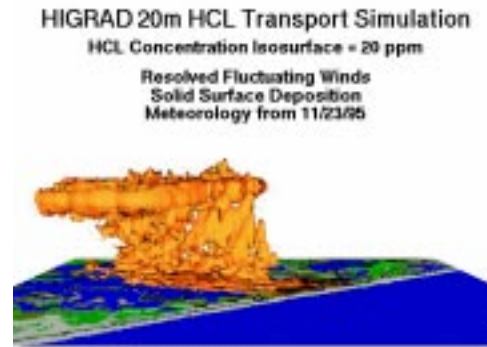
One success has been the emergence of models to simulate the behavior of wildfire. Originally, the EES Division approach was based on combining the operational codes used by the US Forest Service, empirically developed descriptions of the spread rate and heat output of fires in various fuel types, with small-scale meteorology models.

- Recently, this has matured into the inclusion of a full-physics combustion code in an advanced numerical turbulence model. This allows a fully interactive computation between the fire and the local weather. Additional physical processes, such as radiative pre-heating of fuels, smoke emissions, and stochastic descriptions of the branding process (flying, burning embers that start new fires) have also been included in the model.



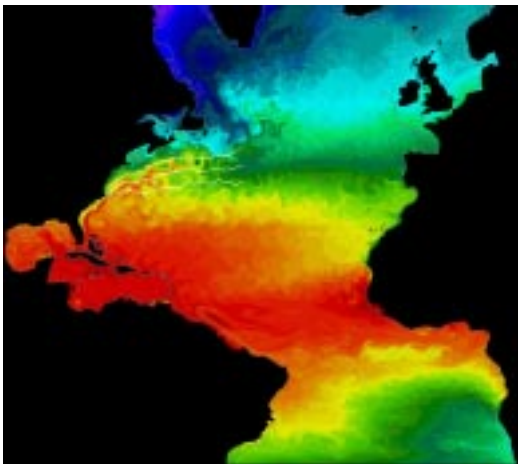
Simulation of the 1994 South Canyon Fire using the LANL HIGRAD meteorology model with the USFS BEHAVE empirical fire model.

- A second area of success in small-scale atmospheric modeling is the application of this code (with the fire turned off) to atmospheric dispersion problems. In 1998, EES scientists showed that concerns about a NASA Space Shuttle abort procedure, raised on the basis of overly simplified plume model computations, were less problematic than originally thought. This year, a new effort with the LANL/DX division is to understand the dispersion of high-explosive test effluents in the complex terrain of the LANL site.
- The model used for these computations is becoming mature enough that there is the potential for commercialization, and this would be a useful direction to explore. An earlier code, originally developed here, is still producing modest royalties for the Laboratory, and the potential of these newer methods would seem significant.



Iso-surfaces of HCl associated with a catastrophic abort procedure of a NASA Space Shuttle launch.

6. Predictive Modeling of Complex Earth and Environmental Systems. This capability centers on predicting the interaction between global, regional, and local systems by understanding the linkages, interfaces, and feedback mechanisms for the flux of mass and energy between them, with and without anthropogenic effects. The capability also encompasses behavior of natural systems that



High-resolution simulation of the N. Atlantic circulation using MICOM. Colors depict surface temperature.

are so complex or large that computational approaches are the preferred way to develop testable hypotheses.

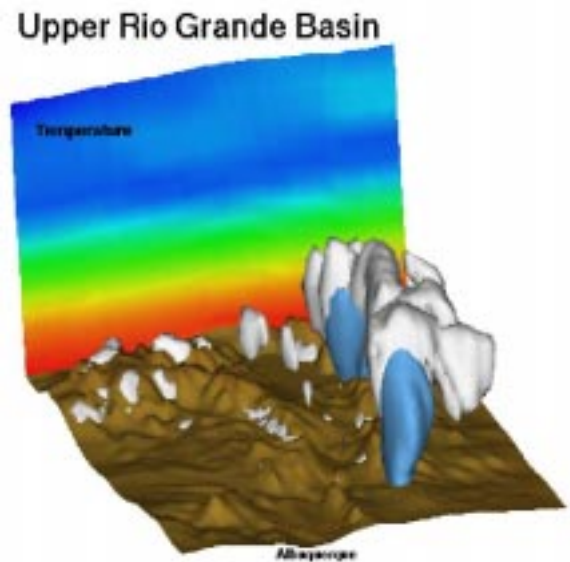
Ocean Circulation Modeling. EES scientists' involvement in larger-scale modeling of the atmosphere and the ocean has grown dramatically over the past year as a result of the merging of the Miami Isopycnic Coordinate Ocean Model (MICOM) and the LANL Parallel Ocean Program (POP). It can be argued that Los Alamos is now the premier ocean circulation-modeling center in the world. The POP has been adopted by the Climate System Model project at National Center for Atmospheric Research for the next generation

coupled global climate model. Future developments (notably, the hybrid combination of POP and MICOM into the Hybrid Coordinate Ocean Circulation Model—HYCOM) will also become modules

in the CSM, making Los Alamos a partner in the de facto US National Climate Modeling effort. When DOE funding becomes available, under the Accelerated Climate Prediction Initiative (ACPI), Los Alamos will join with NCAR and LLNL in a global model development and applications consortium. Another area of potential growth in the LANL ocean modeling effort concerns the Laboratory's capability to do classified computing. MICOM, through the University of Miami, has recently been adopted by the US Navy as its open ocean simulation tool; a five-year center has been established for the purpose of (a) upgrading MICOM (this will be the HYCOM) and (b) developing a real-time data assimilation capability to make deterministic ocean forecasts possible. The computational efficiency, physical faithfulness, and flexibility (including its high-resolution capability) of MICOM make it useful to the Navy for tactical purposes. The potential for LANL is to become a partner with the Navy in its tactical computations.

Simulating Climate Change. In addition to our focus on oceanic modeling, LANL also has a strong capability in atmospheric modeling, particularly on regional scales. Simulations of atmospheric behavior on the scale of individual watersheds, for example, has a strong connection to water resource issues on these scales. The Regional Atmospheric Modeling System (RAMS) has been used to simulate precipitation over the Rio Grandé Valley to show the connection between preferred locations for rain and snowfall and the topography. This study also shows clearly the need for resolution of at least 5 km for correctly simulating these processes.

Precipitation simulation using the RAMS, for the central Rio Grandé Valley.



Simulating the Behavior of the Earth's Magnetic Field. In the mid 1990s, an IGPP-sponsored collaboration solved one of the problems in physics that Albert Einstein listed earlier in the century as remaining to be understood. This problem is how the Earth generates its magnetic field (and its polarity reversals).

- This culminated in 1996 when an EES/IGPP scientist successfully simulated the Earth's Geodynamo in three-dimensional spherical geometry with accurate Earth parameters. He was able to show that the earth's magnetic field originates in its convectively turbulent liquid iron

core. The simulations required the largest computers available both at NSF centers and at Los Alamos. The results were published in *Nature*.

- The chaotic nature of the fluid motions, greatly complicated by the coriolis force due to the Earth's rotation, is the reason for the heretofore-puzzling nature of time-dependent changes (including actual reversals in polarity) in the field. The simulations also predicted that magnetic torques in the Earth's solid iron inner core (about the size of the moon) would cause it to rotate slightly faster than the rest of the Earth. Subsequently this prediction was observed.
- The findings have completely changed the research community's understanding of how planets generate magnetic fields and has caused a new resurgence in field observations, which are increasingly relying on these groundbreaking simulations to guide reduction and analysis of the data.